

Phenylalanine
150-30-1 | DTXSID9023463

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.93	22.5	0.93	22.1	0.93	22.1

Model Results

Predicted value: 287 °C

Global applicability domain: Inside

Local applicability domain index: 2.66e-01

Confidence level: 7.69e-01

Nearest Neighbors from the Training Set

Image not found

Chloramben

Measured: 312

Predicted: 301

Image not found

4-Phenylbutyric acid

Measured: 290

Predicted: 276